

<b>Experiment title:</b> Determination of the partial structure factors in the amorphous Blue-Ray-Disc storage material $\text{Ge}_8\text{Sb}_2\text{Te}_{11}$ and in $\text{Ge}_2\text{Sb}_2\text{Te}_4$	<b>Experiment number:</b> HD 510
<b>Beamline:</b>	<b>Date of report:</b> 23.02.2012
<b>Shifts:</b>	<b>Date of experiment:</b> from: 14.11.2011 to: 22.11.2011  <b>Local contact(s):</b> J.-F. Berar and N. Boudet

**Names and affiliations of applicants** (\* indicates experimentalists):

W.C. Pilgrim\*, S. Hosokawa\*, Jens Stelhorn\*, Astrid Höhle

Physical Chemistry,

Philipps-University of Marburg, 35032 Marburg,

Germany

**Report:**

We are currently aiming to explore the structural properties of different amorphous Ge-Te-Sb alloys. In their ternary phase diagram these compounds lie on the so called *tie-line* - the

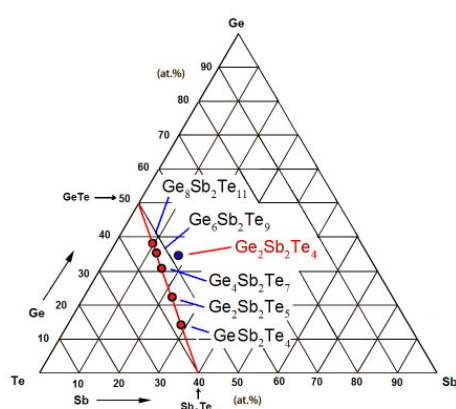


Fig. 1: Ternary Ge-Sb-Te phase diagram. Red line: pseudo binary line of the GeTe-Sb<sub>3</sub>Te<sub>2</sub>-system (tie-line).

pseudo binary conjunction between GeTe and Sb<sub>2</sub>Te<sub>3</sub> (see Fig.1). All members of this group are known to be excellent Phase Change Materials (PCMs), i.e. they can reversibly switch back and forth between a polycrystalline and an amorphous phase on the nanosecond scale, thereby also changing their optical properties. The latter is utilized for optical data storage and some members of this group are already commercially employed in the production of optical storage devices. However, the origin of this remarkable behaviour is yet not fully understood. In the crystalline phase these materials show some characteristic trends with increasing Ge-content (from bottom to top along the tie-line). The number of free electrons increases and the optical

contrast between the phases rises. Additionally, the number of vacancies in the crystals decreases and related structural variations are observed. The question is whether such variations are also seen in the respective amorphous phases. The structural properties of these compounds were so far explored using conventional x-ray diffraction and EXAFS. Some characteristic structural information exists about the crystals, but much less is known about

the amorphous phases. This is due to the difficulties in exploring and describing amorphous multicomponent systems where all partial correlation functions must be accurately known in order to unambiguously determine atomic distances and coordination numbers. In a three component system, the number of partials amounts to six and it is virtually impossible to determine them directly from experiment. Therefore we decided to explore the amorphous phases using Anomalous X-Ray Scattering. This allows determining the differential scattering laws  $\Delta_i S(Q)$  containing all correlations of atomic sort  $i$  to all constituents of the sample. These three functions together with the total  $S(Q)$  are then employed in a subsequent RMC-analysis. This is yet the most reliable procedure to obtain partial structural information of a multicomponent amorphous system from RMC.

It was intended to measure a-Ge<sub>8</sub>Sb<sub>2</sub>Te<sub>11</sub> for comparison with earlier a-Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub>-results. In order to explore the influence of crystal vacancies on the amorphous structure it was also planned to determine the  $\Delta_i S(Q)$  of a-Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>4</sub>, which forms a vacancy free crystal. It is not situated on the *tie-line* (see Fig. 1). Unfortunately, we encountered severe sample problems. While a-Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>4</sub> turned out to be fully crystallized after preparation, the a-Ge<sub>8</sub>Sb<sub>2</sub>Te<sub>11</sub>-sample appeared to be heavily contaminated with polycarbonate which was used as substrate in the production process. Despite the contamination we measured the  $\Delta_i S(Q)$  of a-Ge<sub>8</sub>Sb<sub>2</sub>Te<sub>11</sub> and spent the remaining time for test measurements on another *tie-line* member: a-GeTe. Since a-GeTe was also prepared on polycarbonate substrates, we found the same contamination there. In order to nevertheless obtain reasonable data, we measured the scattering from a pure polycarbonate disk in a subsequent experiment using conventional inhouse x-ray scattering. After subtracting the polycarbonate scattering appropriately and after applying the usual corrections, we could obtain reasonable total and differential scattering laws for the two samples. A detailed data treatment to obtain reliable data on a quantitative basis is still in progress. Fig. 2 shows some exemplary preliminary results for a-Ge<sub>8</sub>Sb<sub>2</sub>Te<sub>11</sub> (Fig 2a) and a-GeTe (Fig 2b).

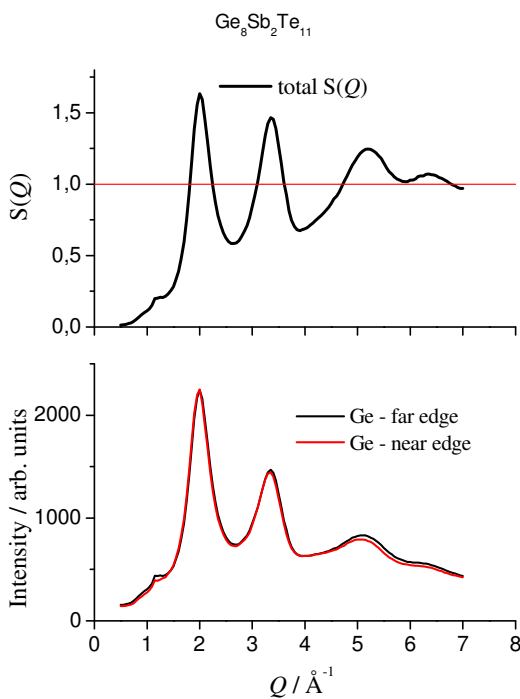


Fig. 2a: total  $S(Q)$  for a-Ge<sub>8</sub>Sb<sub>2</sub>Te<sub>11</sub> (top). The graph at bottom depicts far- and near-edge measurements at the Ge-K-edge. The difference between the measurements is clearly visible.

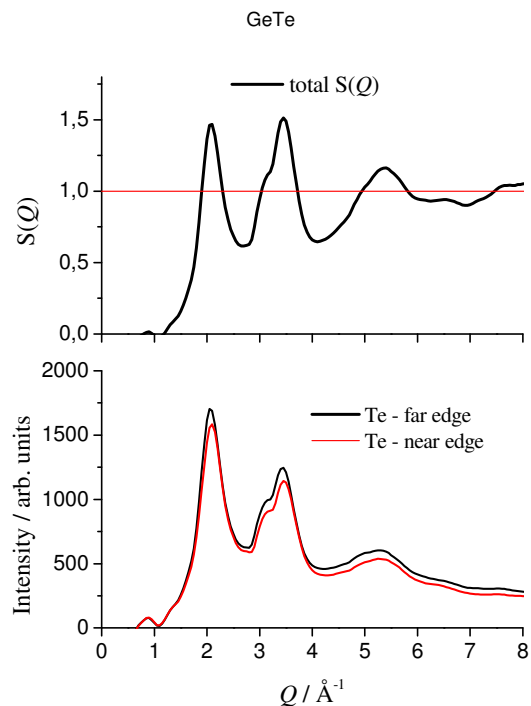


Fig. 2b: total  $S(Q)$  for a-GeTe (top). The graph at bottom depicts far- and near-edge measurements at the Te-K-edge. The difference between the measurements is clearly visible.